



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:39 PM EDT

PDB ID : 5S4W
Title : Tubulin-Z1416571195-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

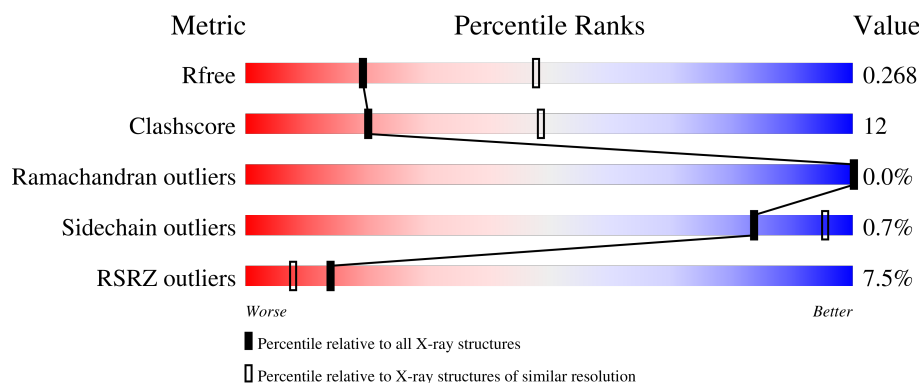
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	C	451	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>.</div> </div> </div>
2	D	445	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MES	B	504	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17775 atoms, of which 13 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	2	1	0
			3359	2109	577	646	27			
2	D	431	Total	C	N	O	S	6	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

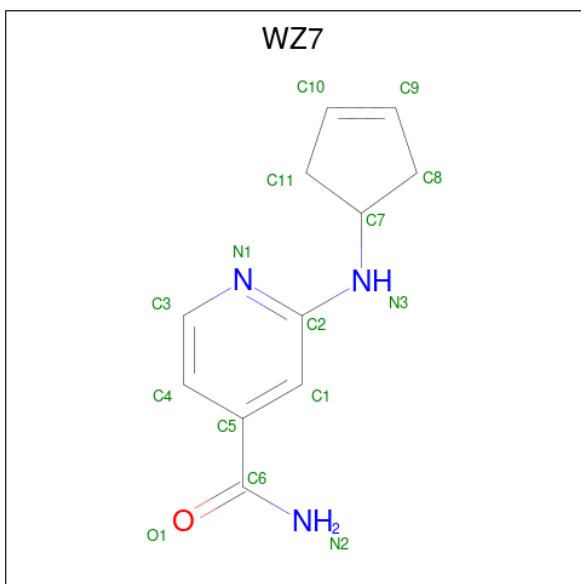
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





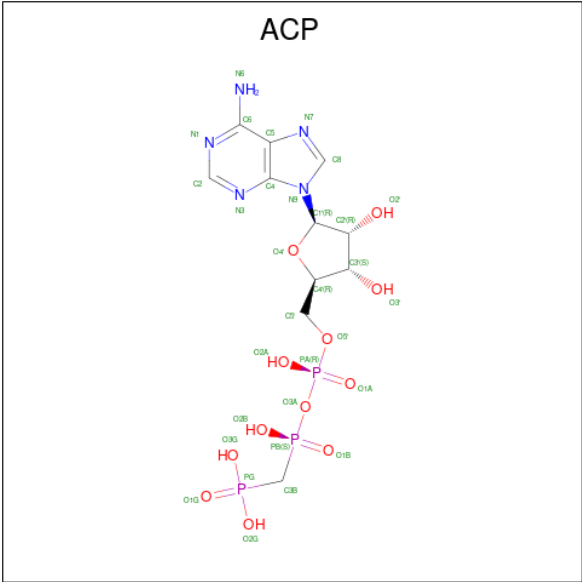
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 2-[(cyclopent-3-en-1-yl)amino]pyridine-4-carboxamide (three-letter code: WZ7) (formula: $C_{11}H_{13}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			28	11	13	3	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

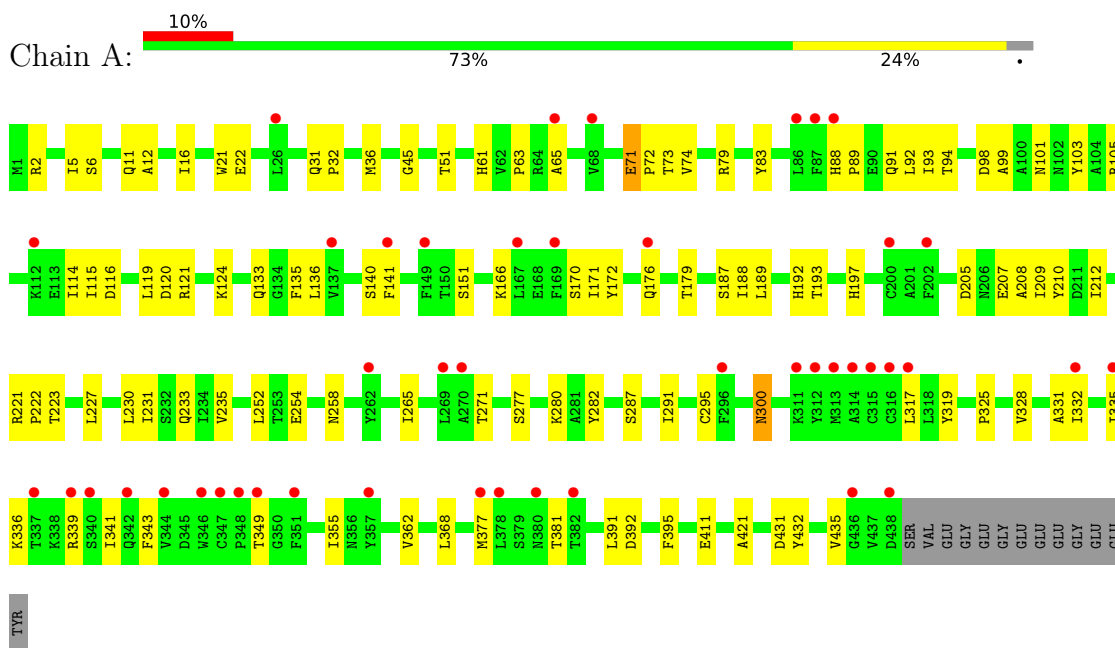
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	12	Total	O	0	0
			12	12		
12	B	26	Total	O	0	0
			26	26		
12	C	43	Total	O	0	0
			43	43		
12	D	6	Total	O	0	0
			6	6		
12	E	3	Total	O	0	0
			3	3		

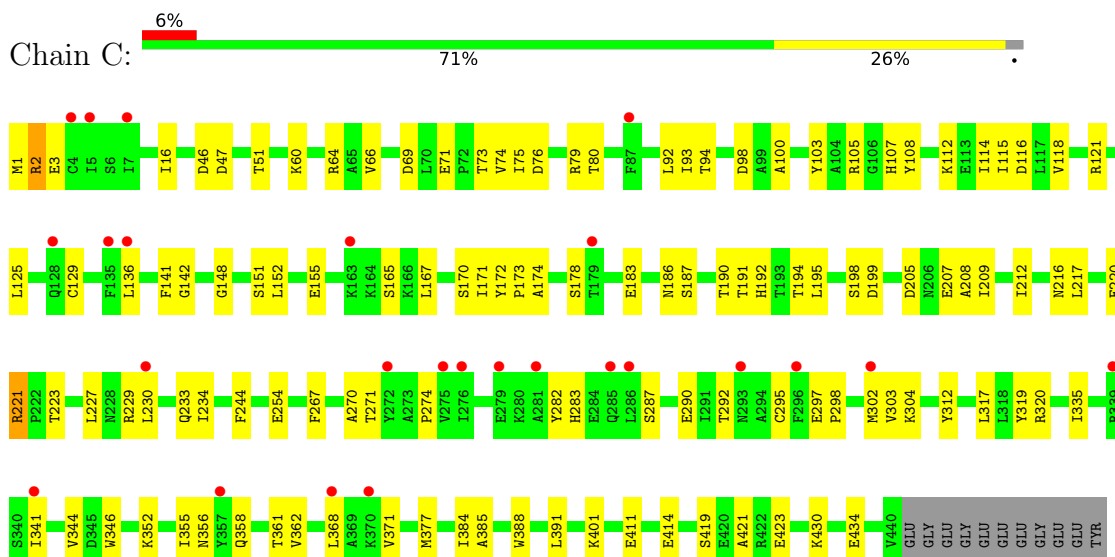
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

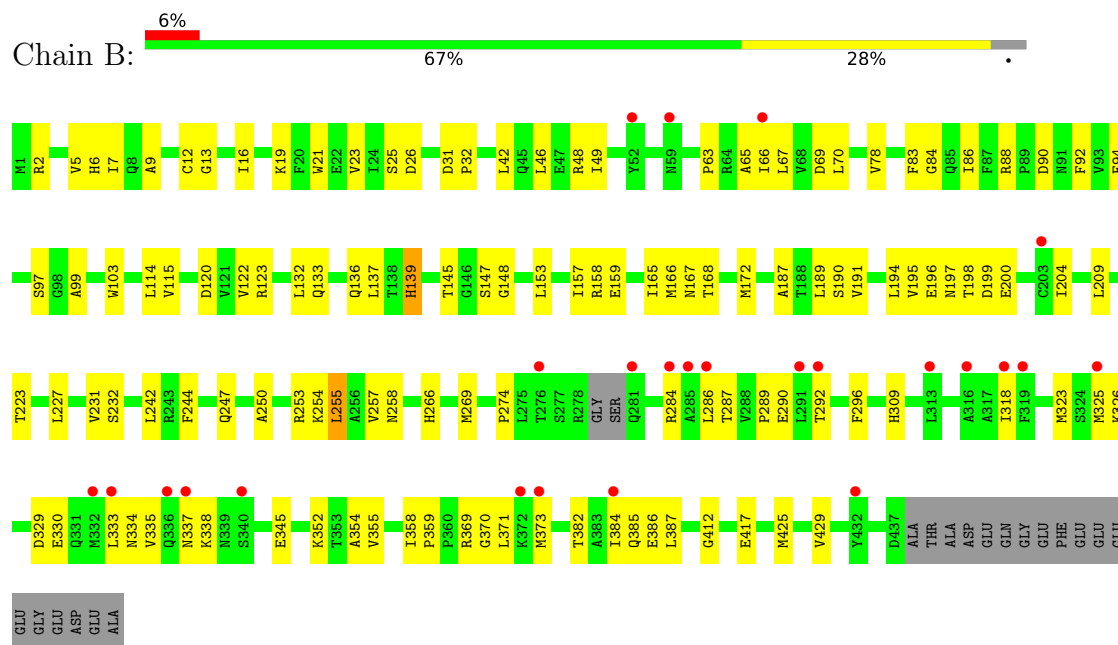
- Molecule 1: Tubulin alpha-1B chain



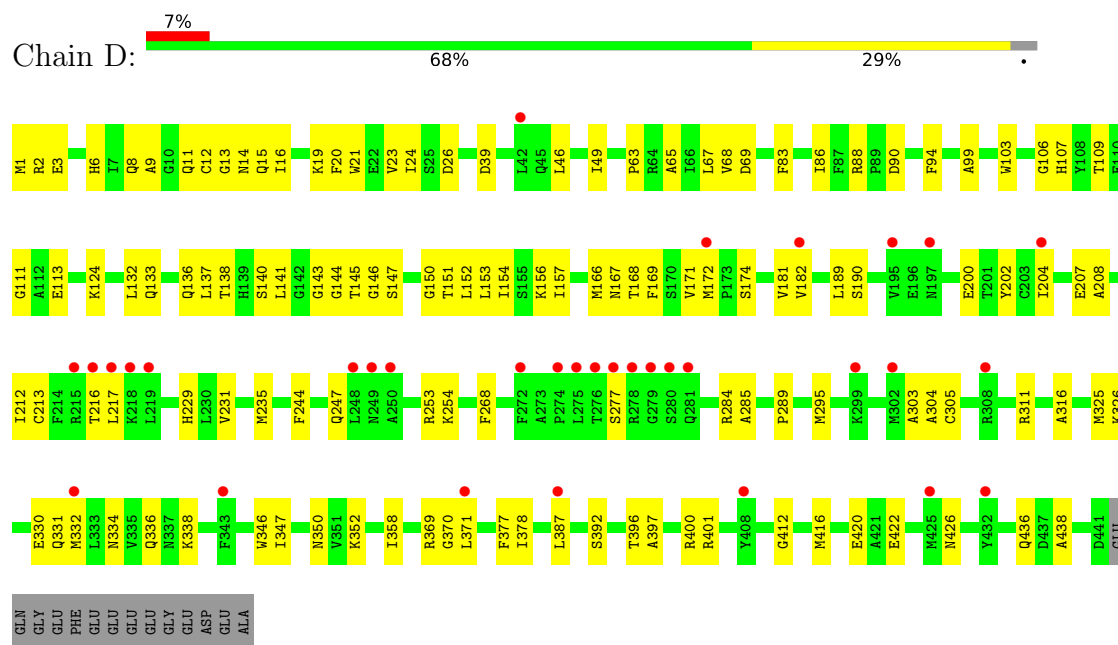
- Molecule 1: Tubulin alpha-1B chain



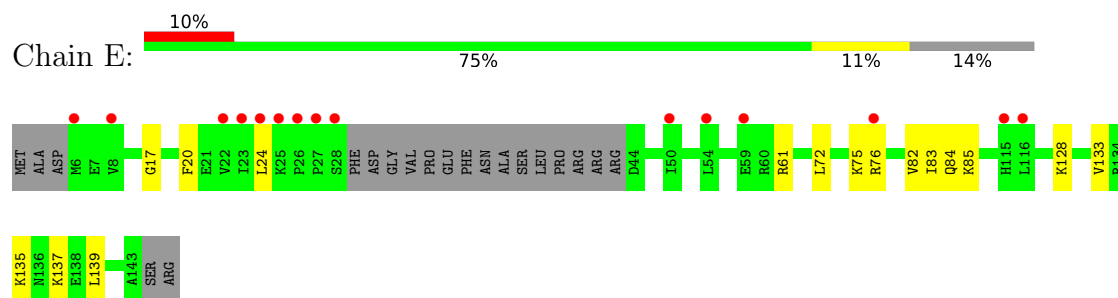
• Molecule 2: Tubulin beta-2B chain



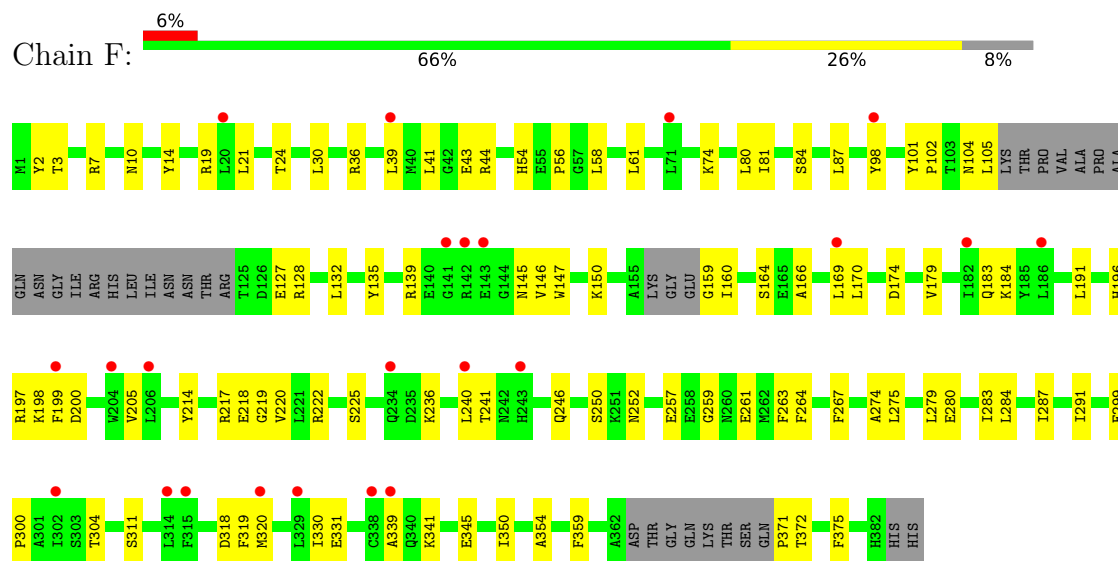
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.13Å 160.08Å 178.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.66 – 2.80 119.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.66-2.80) 98.3 (119.25-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.221 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	3721 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17775	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, WZ7, MG, GDP, ACP, MES, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3433	0.42	0/4647
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.39	0/3978
All	All	0.25	0/17864	0.41	0/24179

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	77	0
1	C	3443	0	3352	99	0
2	B	3359	0	3235	100	0
2	D	3368	0	3236	91	0
3	E	1014	0	1029	16	0
4	F	2877	0	2839	74	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	3	0
9	B	12	0	12	7	0
10	B	15	13	0	3	0
11	F	31	0	14	5	0
12	A	12	0	0	2	0
12	B	26	0	0	3	0
12	C	43	0	0	7	0
12	D	6	0	0	1	0
12	E	3	0	0	1	0
All	All	17762	13	17099	433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.48	0.92
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.41	0.83
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.43	0.83
4:F:80:LEU:O	4:F:84:SER:OG	1.98	0.81
1:C:178:SER:OG	2:D:352:LYS:NZ	2.14	0.79
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.65	0.79
2:D:217:LEU:HA	2:D:277:SER:HB3	1.64	0.79
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.67	0.77
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.66	0.76
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.33	0.76
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.68	0.75
5:C:501:GTP:O1B	12:C:601:HOH:O	2.04	0.74
2:D:174:SER:OG	2:D:207:GLU:OE1	2.04	0.74
1:C:69:ASP:OD2	12:C:602:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.70	0.73
1:C:229:ARG:NH1	12:C:606:HOH:O	2.21	0.73
2:D:83:PHE:O	2:D:86:ILE:HG22	1.88	0.73
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.05	0.73
2:D:136:GLN:HA	2:D:167:ASN:O	1.88	0.73
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.69	0.73
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.70	0.72
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.73	0.71
2:B:83:PHE:O	2:B:86:ILE:HG22	1.91	0.70
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.21	0.70
2:B:199:ASP:OD1	9:B:504:MES:H62	1.90	0.70
1:C:271:THR:HG21	1:C:295:CYS:O	1.92	0.70
2:B:21:TRP:O	2:B:25:SER:OG	2.02	0.69
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.74	0.68
2:B:417:GLU:O	12:B:601:HOH:O	2.12	0.68
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.27	0.68
2:B:158:ARG:NH2	9:B:504:MES:H52	2.07	0.68
2:D:147:SER:HB2	2:D:190:SER:OG	1.94	0.68
2:B:136:GLN:HA	2:B:167:ASN:O	1.94	0.68
2:D:140:SER:HB2	12:D:601:HOH:O	1.94	0.68
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.29	0.67
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.74	0.67
2:B:370:GLY:O	2:B:371:LEU:HD23	1.95	0.67
2:B:69:ASP:OD1	12:B:602:HOH:O	2.13	0.66
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.94	0.66
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.78	0.66
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.78	0.66
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.77	0.66
2:B:97:SER:HA	1:C:2:ARG:NH1	2.09	0.66
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.78	0.66
2:B:88:ARG:NH1	2:B:90:ASP:OD2	2.29	0.66
1:C:178:SER:HB2	1:C:183:GLU:OE2	1.96	0.66
2:B:354:ALA:HB2	10:B:505:WZ7:C10	2.26	0.66
1:A:166:LYS:HE2	1:A:197:HIS:O	1.96	0.65
2:B:147:SER:HG	2:B:190:SER:HG	1.43	0.65
1:C:165:SER:HA	1:C:199:ASP:OD2	1.95	0.65
2:B:145:THR:HB	8:B:501:GDP:O2B	1.95	0.65
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.32	0.65
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.80	0.64
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.34	0.63
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:O	2:D:23:VAL:HG23	1.99	0.63
1:C:234:ILE:HD13	1:C:302:MET:CE	2.29	0.62
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.22	0.62
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.34	0.62
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.34	0.62
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.64	0.62
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.30	0.62
1:C:186:ASN:O	1:C:190:THR:HG22	1.99	0.61
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.81	0.61
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.00	0.61
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.36	0.61
2:D:200:GLU:HB2	2:D:268:PHE:CE2	2.35	0.61
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.83	0.61
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.82	0.61
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.82	0.60
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.00	0.60
4:F:150:LYS:NZ	4:F:183:GLN:OE1	2.29	0.60
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.00	0.60
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.35	0.60
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.31	0.60
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.35	0.60
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.37	0.60
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.82	0.59
1:C:74:VAL:HB	12:C:608:HOH:O	2.02	0.59
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.66	0.59
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.37	0.59
4:F:304:THR:HG21	4:F:311:SER:OG	2.02	0.59
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.59
2:B:323:MET:HE1	2:B:373:MET:HB2	1.84	0.59
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.85	0.59
2:B:158:ARG:NE	9:B:504:MES:H32	2.17	0.59
2:B:253[B]:ARG:O	2:B:257:VAL:HG23	2.02	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
2:B:69:ASP:O	2:B:94:PHE:HA	2.03	0.59
4:F:320:MET:CG	4:F:330:ILE:HD11	2.32	0.59
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.30	0.59
1:C:244:PHE:HB2	1:C:356:ASN:ND2	2.18	0.58
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.84	0.58
4:F:371:PRO:HA	4:F:372:THR:C	2.21	0.58
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.85	0.58
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:NH1	2:B:196:GLU:O	2.37	0.58
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.38	0.58
1:C:76:ASP:O	1:C:80:THR:HG22	2.03	0.58
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.38	0.58
1:A:431:ASP:O	1:A:435:VAL:HG23	2.04	0.58
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.85	0.58
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.58
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.19	0.57
2:D:141:LEU:HA	2:D:147:SER:HB3	1.86	0.57
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.84	0.57
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.40	0.57
1:A:141:PHE:HB3	1:A:187:SER:OG	2.05	0.57
1:C:47:ASP:OD2	12:C:603:HOH:O	2.17	0.57
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.40	0.57
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.87	0.57
4:F:371:PRO:HA	4:F:372:THR:O	2.05	0.57
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.40	0.56
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.15	0.56
2:B:158:ARG:HH11	2:B:197:ASN:HA	1.71	0.56
9:B:504:MES:H31	12:B:605:HOH:O	2.03	0.56
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.39	0.56
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.20	0.56
2:B:412:GLY:C	3:E:82:VAL:HG13	2.26	0.56
1:C:320:ARG:HA	1:C:356:ASN:O	2.05	0.56
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.36	0.56
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.87	0.56
2:B:46:LEU:HA	2:B:49:ILE:HB	1.88	0.56
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.41	0.56
2:D:392:SER:O	2:D:396:THR:HG22	2.06	0.56
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.86	0.56
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.24	0.55
2:B:242:LEU:HD21	2:B:255:LEU:HD23	1.88	0.55
2:B:359:PRO:HB2	2:B:371:LEU:O	2.07	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.55
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.39	0.55
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.88	0.55
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.36	0.55
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.37	0.55
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.55
1:C:271:THR:CG2	1:C:295:CYS:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.42	0.55
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.36	0.55
4:F:19:ARG:HD2	4:F:19:ARG:O	2.08	0.54
2:B:354:ALA:HB2	10:B:505:WZ7:C9	2.37	0.54
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.07	0.54
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.89	0.54
1:A:328:VAL:O	1:A:332:ILE:HG13	2.06	0.54
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.42	0.54
3:E:135:LYS:O	3:E:139:LEU:HG	2.07	0.54
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.07	0.54
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.90	0.54
2:D:69:ASP:O	2:D:94:PHE:HA	2.08	0.54
2:D:204:ILE:HG21	2:D:231:VAL:HG22	1.89	0.53
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.56	0.53
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.90	0.53
1:A:355:ILE:O	3:E:17:GLY:HA3	2.07	0.53
2:B:158:ARG:HD2	9:B:504:MES:H22	1.90	0.53
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.41	0.53
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.43	0.53
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.89	0.53
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.43	0.53
1:A:151:SER:HB2	1:A:193:THR:OG1	2.09	0.53
4:F:371:PRO:HA	4:F:372:THR:HB	1.90	0.53
1:A:223:THR:HA	2:B:247:GLN:HE22	1.74	0.53
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.91	0.53
2:D:11:GLN:O	2:D:15:GLN:HG2	2.08	0.53
2:D:147:SER:O	2:D:151:THR:HG23	2.09	0.53
2:D:326:LYS:O	2:D:330:GLU:HG3	2.08	0.53
2:B:223:THR:O	2:B:227:LEU:HD13	2.08	0.53
2:B:250:ALA:CB	2:B:254:LYS:HD2	2.38	0.53
2:D:295:MET:CE	2:D:377:PHE:HB2	2.39	0.53
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.44	0.52
4:F:350:ILE:O	4:F:354:ALA:HB3	2.09	0.52
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.44	0.52
1:A:6:SER:O	1:A:65:ALA:HA	2.08	0.52
3:E:72:LEU:O	3:E:76:ARG:HG2	2.10	0.52
4:F:225:SER:O	4:F:252:ASN:HB2	2.08	0.52
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.90	0.52
2:D:397:ALA:O	2:D:401:ARG:NH1	2.43	0.52
1:C:1:MET:O	1:C:2:ARG:HB2	2.10	0.52
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.40	0.52
2:B:318:ILE:N	2:B:318:ILE:HD12	2.25	0.52
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.52
2:D:208:ALA:O	2:D:212:ILE:HG13	2.10	0.52
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.92	0.52
1:A:120:ASP:O	1:A:124:LYS:HG3	2.10	0.52
2:B:382:THR:O	2:B:385:GLN:HG2	2.09	0.52
2:D:146:GLY:O	2:D:150:GLY:HA3	2.10	0.51
2:B:165:ILE:HA	2:B:199:ASP:OD2	2.10	0.51
1:C:271:THR:HG21	1:C:295:CYS:HA	1.92	0.51
1:A:287:SER:O	1:A:291:ILE:HG23	2.10	0.51
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.25	0.51
2:D:145:THR:HB	8:D:501:GDP:O2B	2.10	0.51
2:D:303:ALA:O	2:D:305:CYS:N	2.44	0.51
2:D:311:ARG:NH1	2:D:436:GLN:O	2.42	0.51
4:F:21:LEU:O	4:F:24:THR:OG1	2.26	0.51
4:F:246:GLN:O	4:F:250:SER:HB3	2.09	0.51
1:C:414:GLU:OE2	12:C:604:HOH:O	2.19	0.51
3:E:85:LYS:NZ	12:E:202:HOH:O	2.43	0.51
1:A:99:ALA:HA	1:A:105:ARG:HD3	1.93	0.51
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.93	0.51
1:C:141:PHE:HB2	1:C:173:PRO:HD3	1.93	0.51
1:A:271:THR:HG21	1:A:295:CYS:HA	1.93	0.51
1:C:174:ALA:HB2	1:C:207:GLU:H	1.76	0.51
1:C:297:GLU:OE2	1:C:298:PRO:HD2	2.11	0.51
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.51
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.93	0.50
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.46	0.50
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.94	0.50
2:B:23:VAL:CG2	2:B:232:SER:HB3	2.39	0.50
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.94	0.50
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.47	0.50
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.94	0.50
2:B:287:THR:HB	2:B:289:PRO:HD2	1.92	0.50
2:D:99:ALA:HB1	2:D:144:GLY:HA3	1.94	0.50
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.94	0.50
2:D:412:GLY:C	3:E:133:VAL:HG13	2.31	0.50
2:B:345:GLU:OE1	2:B:345:GLU:N	2.38	0.50
2:D:167:ASN:HD21	2:D:202:TYR:HE2	1.60	0.50
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.46	0.50
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CZ	9:B:504:MES:H52	2.42	0.49
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.47	0.49
2:B:6:HIS:HD2	2:B:65:ALA:HB1	1.77	0.49
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.47	0.49
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.28	0.49
1:C:107:HIS:O	1:C:152:LEU:HD22	2.12	0.49
2:B:187:ALA:O	2:B:191:VAL:HG23	2.13	0.49
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.95	0.49
1:A:2:ARG:O	1:A:51:THR:HG22	2.12	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.13	0.49
2:B:153:LEU:O	2:B:157:ILE:HG13	2.13	0.49
2:D:212:ILE:O	2:D:216:THR:HB	2.13	0.49
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.48
2:B:97:SER:HA	1:C:2:ARG:HH11	1.78	0.48
1:C:105:ARG:HG3	1:C:411:GLU:HG3	1.94	0.48
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.19	0.48
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.95	0.48
2:B:194:LEU:HA	2:B:198:THR:HG23	1.95	0.48
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.49	0.48
1:C:2:ARG:O	1:C:51:THR:HG22	2.14	0.48
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.14	0.48
1:C:100:ALA:HB2	2:D:253:ARG:HD2	1.96	0.48
4:F:191:LEU:HD13	4:F:196:HIS:CD2	2.48	0.48
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.95	0.48
1:C:46:ASP:N	1:C:46:ASP:OD1	2.45	0.47
2:D:181:VAL:HG13	2:D:182:VAL:HG13	1.95	0.47
1:A:317:LEU:CD2	1:A:377:MET:HG3	2.44	0.47
2:B:323:MET:CE	2:B:373:MET:HB2	2.44	0.47
1:C:216:ASN:O	1:C:217:LEU:HD23	2.13	0.47
2:B:329:ASP:O	2:B:333:LEU:HG	2.14	0.47
4:F:150:LYS:HD2	11:F:401:ACP:O2A	2.13	0.47
1:A:71:GLU:HG2	1:A:73:THR:H	1.80	0.47
2:B:191:VAL:O	2:B:195:VAL:HG23	2.15	0.47
1:C:107:HIS:CD2	1:C:152:LEU:HB2	2.50	0.47
1:A:176:GLN:HG3	4:F:56:PRO:HG3	1.96	0.47
1:A:208:ALA:O	1:A:212:ILE:HG13	2.14	0.47
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.95	0.47
1:C:114:ILE:HG12	1:C:118:VAL:HG23	1.97	0.47
1:A:176:GLN:HG3	4:F:56:PRO:CG	2.44	0.47
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.95	0.47
1:C:270:ALA:O	1:C:302:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:O	1:A:231:ILE:HG13	2.15	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.47
2:D:9:ALA:HA	2:D:68:VAL:O	2.15	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.47
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.97	0.47
2:D:11:GLN:N	8:D:501:GDP:O1B	2.27	0.47
2:D:284:ARG:O	2:D:285:ALA:HB3	2.15	0.47
4:F:259:GLY:O	4:F:261:GLU:HG3	2.15	0.47
1:A:72:PRO:HA	1:A:94:THR:CG2	2.46	0.46
2:B:269:MET:HG2	2:B:384:ILE:HD13	1.96	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
2:D:107:HIS:O	2:D:152:LEU:HD22	2.15	0.46
2:D:153:LEU:O	2:D:157:ILE:HG13	2.14	0.46
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.50	0.46
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.47	0.46
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.97	0.46
1:C:317:LEU:HD23	1:C:377:MET:HG3	1.97	0.46
2:D:12:CYS:O	2:D:16:ILE:HG12	2.16	0.46
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.81	0.46
2:B:412:GLY:O	3:E:82:VAL:HG13	2.16	0.46
1:C:192:HIS:CG	1:C:421:ALA:HA	2.50	0.46
1:C:230:LEU:O	1:C:234:ILE:HD12	2.15	0.46
1:C:419:SER:O	1:C:423:GLU:HG3	2.15	0.46
2:D:422:GLU:HG2	2:D:426:ASN:HD21	1.80	0.46
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.98	0.46
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.26	0.46
1:C:191:THR:O	1:C:195:LEU:HB2	2.15	0.46
1:A:115:ILE:O	1:A:119:LEU:HG	2.16	0.46
2:B:326:LYS:O	2:B:330:GLU:HG3	2.16	0.46
1:C:208:ALA:O	1:C:212:ILE:HG13	2.15	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.46
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.50	0.46
2:B:334:ASN:O	2:B:338:LYS:HG3	2.16	0.46
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.97	0.46
4:F:7:ARG:HE	4:F:43:GLU:CD	2.17	0.46
1:A:411:GLU:O	3:E:61:ARG:NH1	2.39	0.46
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.98	0.45
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.51	0.45
4:F:39:LEU:HD12	4:F:61:LEU:O	2.14	0.45
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.16	0.45
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:135:TYR:OH	4:F:139:ARG:NH2	2.48	0.45
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.99	0.45
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.46	0.45
2:B:9:ALA:O	2:B:13:GLY:HA3	2.17	0.45
2:B:199:ASP:O	2:B:266:HIS:HB2	2.16	0.45
3:E:128:LYS:O	3:E:128:LYS:HD3	2.17	0.45
4:F:98:TYR:HA	4:F:127:GLU:OE1	2.16	0.45
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.51	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.17	0.45
1:C:287:SER:OG	1:C:290:GLU:HG3	2.17	0.45
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.82	0.45
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.52	0.45
1:A:115:ILE:HG23	1:A:116:ASP:N	2.32	0.44
1:A:179:THR:HA	2:B:352:LYS:HD2	1.99	0.44
1:C:174:ALA:O	1:C:178:SER:HB3	2.17	0.44
1:C:267:PHE:O	1:C:384:ILE:HD13	2.16	0.44
2:D:370:GLY:O	2:D:371:LEU:HD23	2.17	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.98	0.44
2:D:2:ARG:C	2:D:133:GLN:HE21	2.21	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.44
2:B:42:LEU:H	2:B:42:LEU:HD12	1.82	0.44
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.99	0.44
2:B:158:ARG:HD2	9:B:504:MES:C2	2.48	0.44
1:A:99:ALA:HA	1:A:105:ARG:CD	2.48	0.44
1:A:331:ALA:O	1:A:335:ILE:HG13	2.17	0.44
1:C:151:SER:O	1:C:155:GLU:HG3	2.18	0.44
2:D:9:ALA:O	2:D:13:GLY:HA3	2.18	0.44
2:D:289:PRO:HG3	2:D:331:GLN:NE2	2.33	0.44
1:C:108:TYR:O	1:C:112:LYS:HG2	2.18	0.44
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.53	0.44
1:C:282:TYR:O	1:C:283:HIS:HB2	2.17	0.43
4:F:101:TYR:CE2	4:F:179:VAL:HG22	2.53	0.43
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.40	0.43
1:A:5:ILE:O	1:A:135:PHE:HA	2.18	0.43
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.48	0.43
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.01	0.43
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.43
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.53	0.43
1:C:100:ALA:CB	2:D:253:ARG:HD2	2.48	0.43
4:F:198:LYS:HG2	4:F:199:PHE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG12	1:A:114:ILE:O	2.18	0.43
1:C:209:ILE:HD11	1:C:302:MET:CE	2.48	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.53	0.43
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.53	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.43
1:C:234:ILE:HD13	1:C:302:MET:HE2	1.98	0.43
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.53	0.43
1:A:362:VAL:HG22	12:A:604:HOH:O	2.18	0.43
2:B:425:MET:O	2:B:429:VAL:HG23	2.19	0.43
1:C:173:PRO:HG2	1:C:391:LEU:HD11	2.00	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.54	0.43
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.54	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.00	0.43
1:C:223:THR:O	1:C:227:LEU:HG	2.19	0.43
2:D:141:LEU:HD12	2:D:172:MET:SD	2.59	0.43
2:D:332:MET:O	2:D:336:GLN:HG3	2.19	0.42
4:F:371:PRO:N	4:F:372:THR:HB	2.34	0.42
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.54	0.42
1:A:136:LEU:HD21	1:A:252:LEU:HD21	2.01	0.42
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.49	0.42
2:B:115:VAL:HG23	2:B:153:LEU:HD23	2.02	0.42
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.55	0.42
2:B:120:ASP:HA	2:B:123:ARG:NH1	2.35	0.42
1:C:198:SER:HB3	12:C:613:HOH:O	2.19	0.42
1:C:361:THR:HG22	1:C:362:VAL:H	1.85	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.02	0.42
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.02	0.42
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.50	0.42
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.02	0.42
2:D:154:ILE:CG2	2:D:166:MET:HG2	2.49	0.42
3:E:75:LYS:HD3	3:E:76:ARG:NH2	2.35	0.42
4:F:205:VAL:HG21	4:F:291:ILE:CG2	2.48	0.42
1:A:319:TYR:HB2	1:A:355:ILE:HG12	2.01	0.42
2:B:120:ASP:HA	2:B:123:ARG:HH12	1.84	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
2:B:167:ASN:ND2	2:B:200:GLU:HB2	2.35	0.42
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.49	0.42
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.42
1:C:401:LYS:HE2	2:D:438:ALA:HB1	2.01	0.42
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.55	0.42
4:F:274:ALA:CB	4:F:275:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.41
1:C:115:ILE:HG23	1:C:116:ASP:N	2.35	0.41
1:C:174:ALA:HB2	1:C:207:GLU:N	2.35	0.41
1:C:194:THR:O	1:C:194:THR:HG22	2.20	0.41
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.39	0.41
1:A:99:ALA:C	1:A:105:ARG:HD3	2.41	0.41
1:C:207:GLU:HG2	1:C:304:LYS:HD2	2.01	0.41
1:C:220:GLU:HB3	2:D:326:LYS:HD2	2.03	0.41
1:A:277:SER:O	1:A:280:LYS:HB2	2.21	0.41
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.01	0.41
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.56	0.41
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.55	0.41
4:F:3:THR:HB	4:F:30:LEU:HD11	2.01	0.41
4:F:184:LYS:O	11:F:401:ACP:N6	2.51	0.41
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.49	0.41
2:B:78:VAL:O	2:B:84:GLY:HA3	2.20	0.41
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.36	0.41
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.36	0.41
2:D:416:MET:O	2:D:420:GLU:HG3	2.21	0.41
1:A:45:GLY:HA3	12:A:606:HOH:O	2.20	0.41
2:D:152:LEU:O	2:D:156:LYS:HG2	2.21	0.41
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.01	0.41
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.55	0.41
1:A:271:THR:HG23	1:A:300:ASN:HD22	1.84	0.41
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.02	0.41
2:B:325:MET:HE1	2:B:355:VAL:HB	2.03	0.41
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.36	0.41
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.00	0.41
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.56	0.41
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.21	0.41
2:D:67:LEU:HD12	2:D:67:LEU:N	2.36	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.41
1:C:3:GLU:OE1	1:C:129:CYS:HB3	2.21	0.41
2:D:3:GLU:O	2:D:132:LEU:HD12	2.20	0.41
3:E:83:ILE:HG23	3:E:84:GLN:N	2.36	0.41
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.03	0.40
1:C:271:THR:HG22	1:C:295:CYS:HA	2.02	0.40
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.51	0.40
2:D:1:MET:HB3	2:D:1:MET:HE2	1.83	0.40
4:F:240:LEU:HD12	4:F:240:LEU:N	2.37	0.40
4:F:275:LEU:HD22	4:F:275:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.51	0.40
2:D:83:PHE:HB3	2:D:86:ILE:CG2	2.52	0.40
2:D:109:THR:O	2:D:113:GLU:HG2	2.21	0.40
4:F:19:ARG:HD2	4:F:19:ARG:C	2.42	0.40
2:B:13:GLY:CA	2:B:139:HIS:HA	2.51	0.40
2:D:143:GLY:O	2:D:147:SER:OG	2.37	0.40
2:B:255:LEU:HG	10:B:505:WZ7:C5	2.52	0.40
1:C:60:LYS:HE3	1:C:60:LYS:HB2	1.91	0.40
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	415 (95%)	21 (5%)	0	100	100
1	C	439/451 (97%)	423 (96%)	16 (4%)	0	100	100
2	B	422/445 (95%)	401 (95%)	21 (5%)	0	100	100
2	D	429/445 (96%)	410 (96%)	18 (4%)	1 (0%)	47	78
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	326 (95%)	18 (5%)	0	100	100
All	All	2189/2319 (94%)	2093 (96%)	95 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	304	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	364 (99%)	5 (1%)	67	90
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	96
2	B	368/383 (96%)	365 (99%)	3 (1%)	81	94
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	94
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1889 (99%)	13 (1%)	84	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	300	ASN
1	A	381	THR
2	B	48	ARG
2	B	139	HIS
2	B	255	LEU
1	C	2	ARG
1	C	221	ARG
2	D	39	ASP
2	D	229	HIS
2	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	88	HIS
1	A	101	ASN
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	300	ASN
2	B	15	GLN
2	B	167	ASN
2	B	247	GLN
2	B	294	GLN
1	C	133	GLN
1	C	372	GLN
2	D	294	GLN
3	E	103	GLN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GDP	D	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.91	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	C	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.73	6 (18%)
9	MES	B	504	-	12,12,12	2.27	1 (8%)	14,16,16	2.00	6 (42%)
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.49	4 (12%)
10	WZ7	B	505	-	16,16,16	1.52	4 (25%)	19,21,21	1.68	4 (21%)
8	GDP	B	501	6	24,30,30	1.21	2 (8%)	31,47,47	1.99	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	504	-	-	5/6/14/14	0/1/1/1
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
10	WZ7	B	505	-	-	0/8/15/15	0/2/2/2
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.61	1.66	1.77
8	B	501	GDP	C6-C5	4.42	1.49	1.41
8	D	501	GDP	C6-C5	4.12	1.48	1.41
5	A	501	GTP	C6-N1	3.19	1.38	1.33
10	B	505	WZ7	C6-N2	3.12	1.38	1.33
5	C	501	GTP	C6-N1	3.12	1.38	1.33
11	F	401	ACP	PG-O3G	2.92	1.61	1.54
11	F	401	ACP	PG-O2G	2.90	1.61	1.54
10	B	505	WZ7	C2-N1	2.85	1.39	1.34
10	B	505	WZ7	C3-N1	2.84	1.40	1.34
11	F	401	ACP	PB-O3A	2.84	1.61	1.58
11	F	401	ACP	C5-C4	2.54	1.47	1.40
8	D	501	GDP	C5-C4	2.41	1.47	1.40
8	B	501	GDP	C5-C4	2.39	1.47	1.40
10	B	505	WZ7	C4-C5	2.36	1.43	1.39
11	F	401	ACP	PB-O2B	2.24	1.61	1.56

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.34	120.10	127.22
5	A	501	GTP	N3-C2-N1	-5.14	120.37	127.22
8	B	501	GDP	C2-N3-C4	5.08	121.16	115.36
8	D	501	GDP	C2-N3-C4	4.81	120.85	115.36
11	F	401	ACP	PA-O3A-PB	-4.26	119.04	132.56
8	B	501	GDP	C6-C5-C4	-4.23	116.76	120.80
9	B	504	MES	C5-N4-C3	4.22	118.32	108.83
5	C	501	GTP	C2-N3-C4	4.18	120.13	115.36
5	A	501	GTP	C2-N3-C4	4.17	120.11	115.36
8	B	501	GDP	C6-N1-C2	4.17	122.55	115.93
8	D	501	GDP	C5-C6-N1	-4.11	117.81	123.43
8	D	501	GDP	C6-N1-C2	3.97	122.23	115.93
8	B	501	GDP	C5-C6-N1	-3.89	118.11	123.43
8	D	501	GDP	PA-O3A-PB	-3.55	120.65	132.83
11	F	401	ACP	C3'-C2'-C1'	3.52	106.28	100.98
8	B	501	GDP	N3-C2-N1	-3.50	122.56	127.22
8	D	501	GDP	C6-C5-C4	-3.47	117.49	120.80
10	B	505	WZ7	C4-C3-N1	-3.46	119.66	123.96
10	B	505	WZ7	O1-C6-N2	-3.40	117.75	122.58
8	D	501	GDP	N3-C2-N1	-3.15	123.02	127.22
11	F	401	ACP	N3-C2-N1	-3.14	123.78	128.68
8	B	501	GDP	C4-C5-N7	-3.10	106.17	109.40
5	C	501	GTP	C5-C6-N1	-3.02	119.30	123.43
5	A	501	GTP	C5-C6-N1	-3.00	119.32	123.43
5	C	501	GTP	PB-O3B-PG	-2.83	123.13	132.83
9	B	504	MES	C6-C5-N4	-2.77	105.90	110.10
5	C	501	GTP	PA-O3A-PB	-2.77	123.31	132.83
8	B	501	GDP	PA-O3A-PB	-2.76	123.35	132.83
8	D	501	GDP	C4-C5-N7	-2.72	106.56	109.40
5	A	501	GTP	PA-O3A-PB	-2.65	123.75	132.83
5	C	501	GTP	C6-N1-C2	2.62	120.10	115.93
11	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
5	A	501	GTP	C6-N1-C2	2.49	119.88	115.93
9	B	504	MES	O3S-S-C8	2.44	109.71	105.77
5	A	501	GTP	PB-O3B-PG	-2.40	124.60	132.83
9	B	504	MES	C7-N4-C5	2.31	117.14	111.23
8	B	501	GDP	C3'-C2'-C1'	2.27	104.40	100.98
10	B	505	WZ7	O1-C6-C5	2.26	122.34	119.63
9	B	504	MES	O2S-S-C8	2.24	109.62	106.92
9	B	504	MES	O1S-S-C8	2.23	109.59	106.92
10	B	505	WZ7	C11-C7-N3	-2.16	108.12	112.31

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	N4-C7-C8-S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-O3A-PA-O1A
8	B	501	GDP	PA-O3A-PB-O2B
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
9	B	504	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

7 monomers are involved in 22 short contacts:

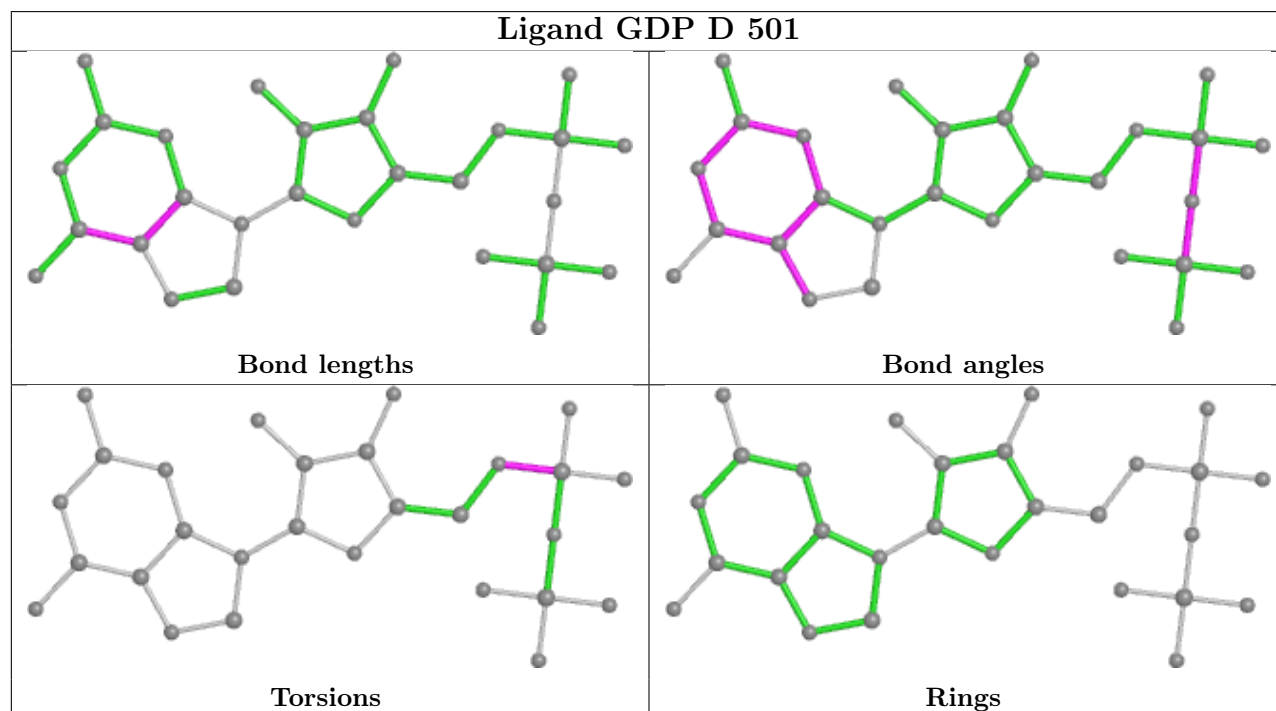
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	3	0

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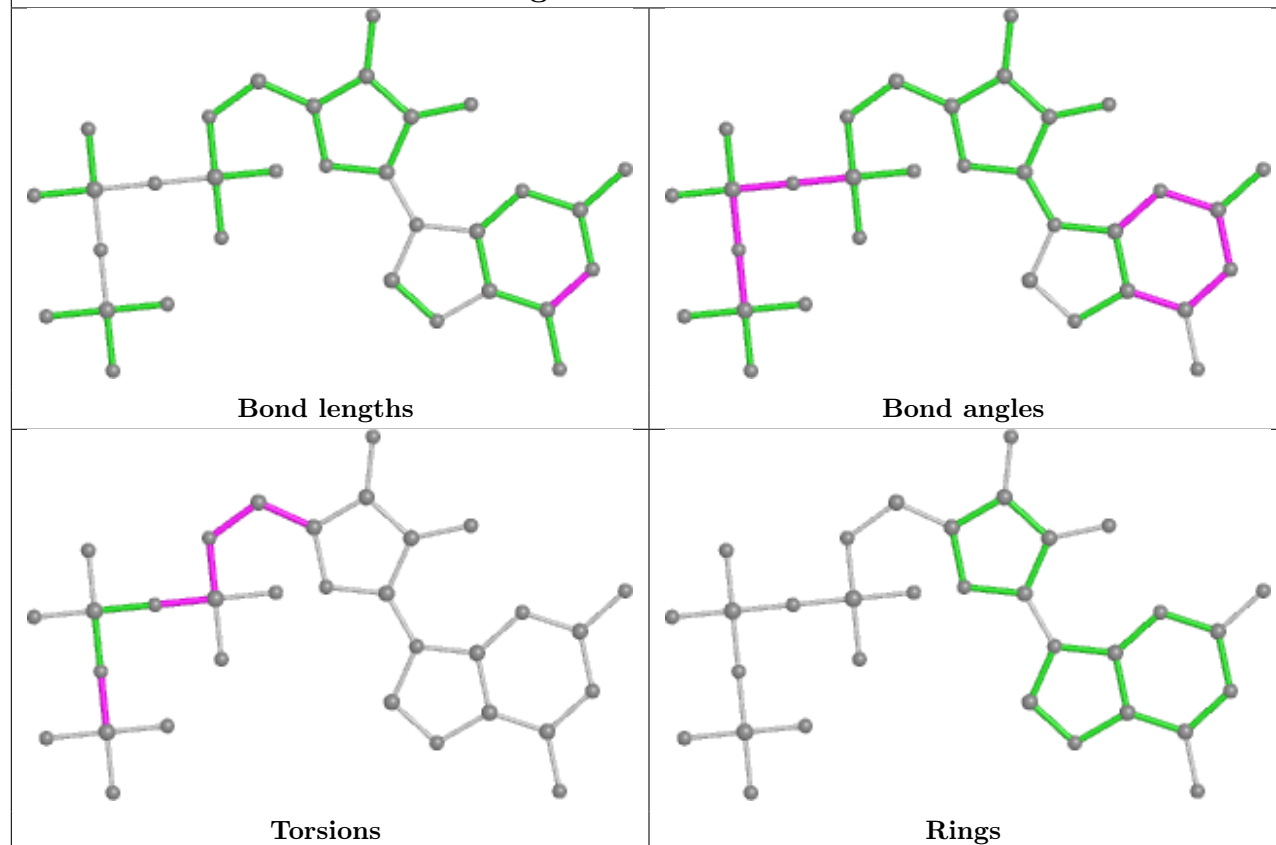
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
5	C	501	GTP	1	0
9	B	504	MES	7	0
11	F	401	ACP	5	0
10	B	505	WZ7	3	0
8	B	501	GDP	2	0

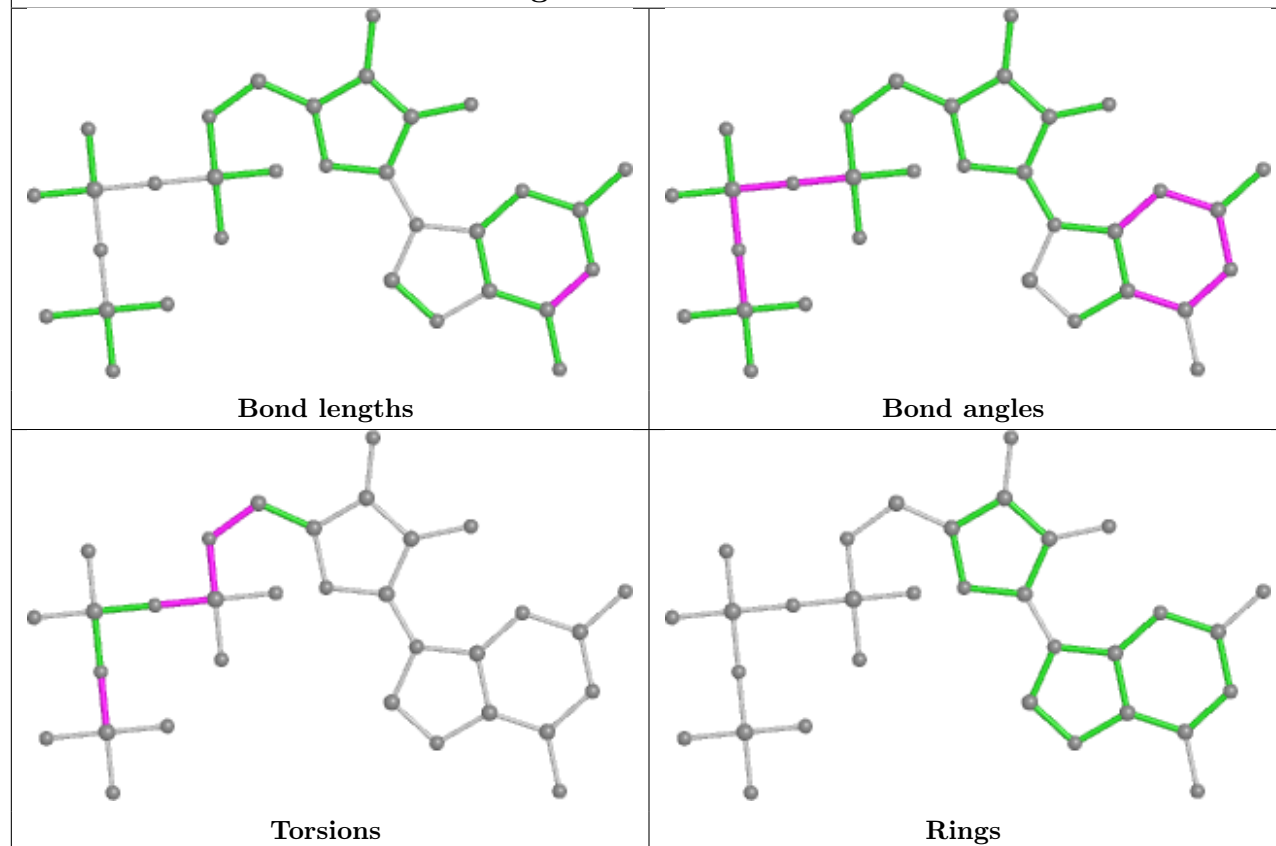
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



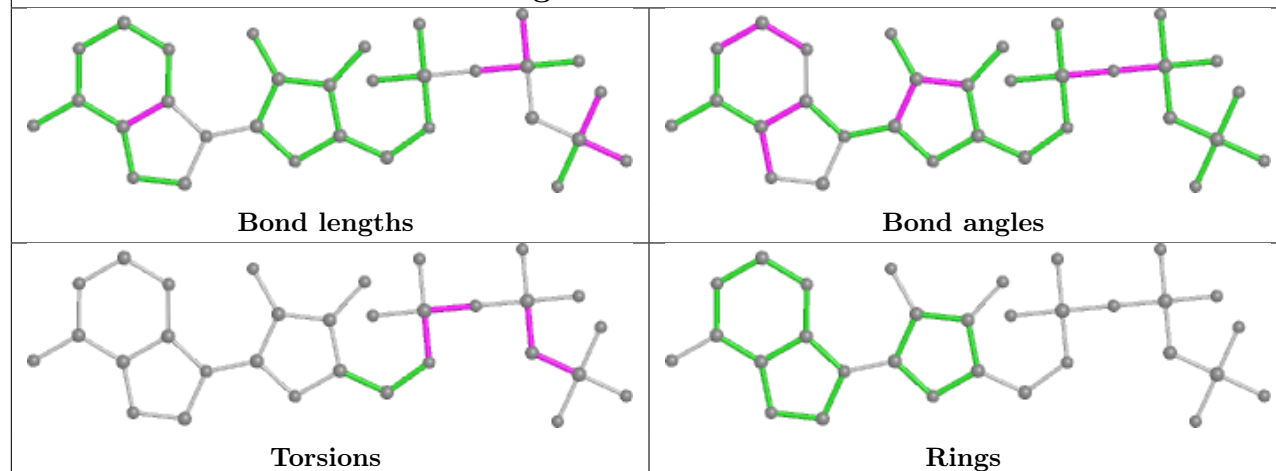
Ligand GTP A 501



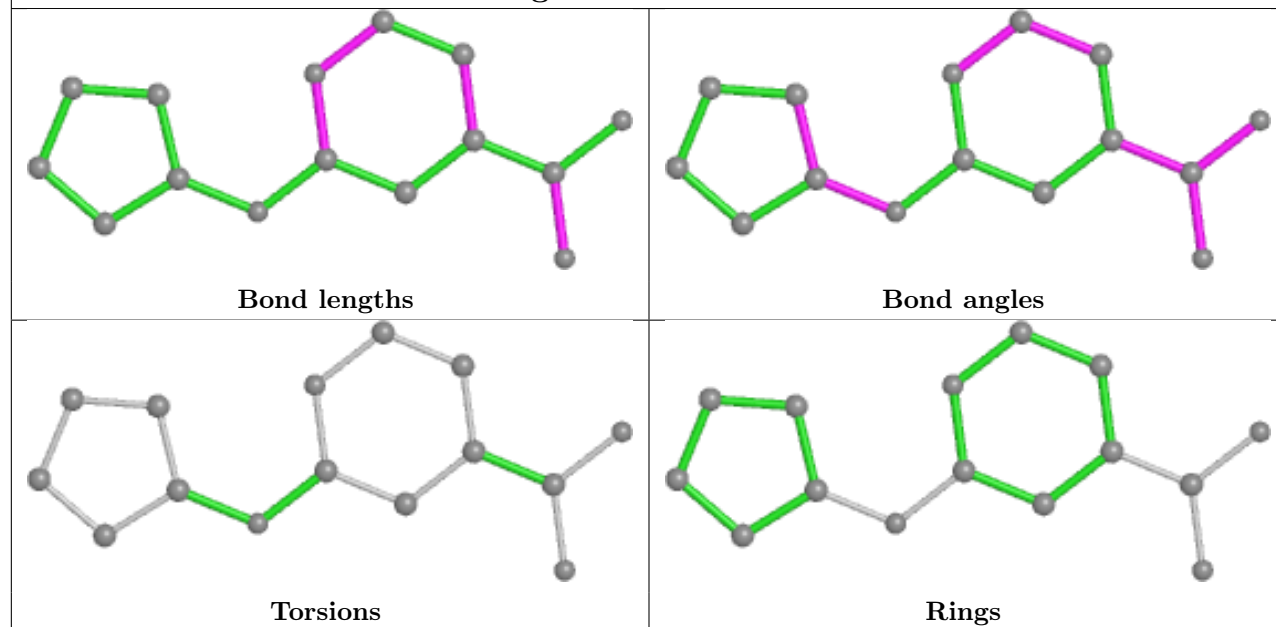
Ligand GTP C 501

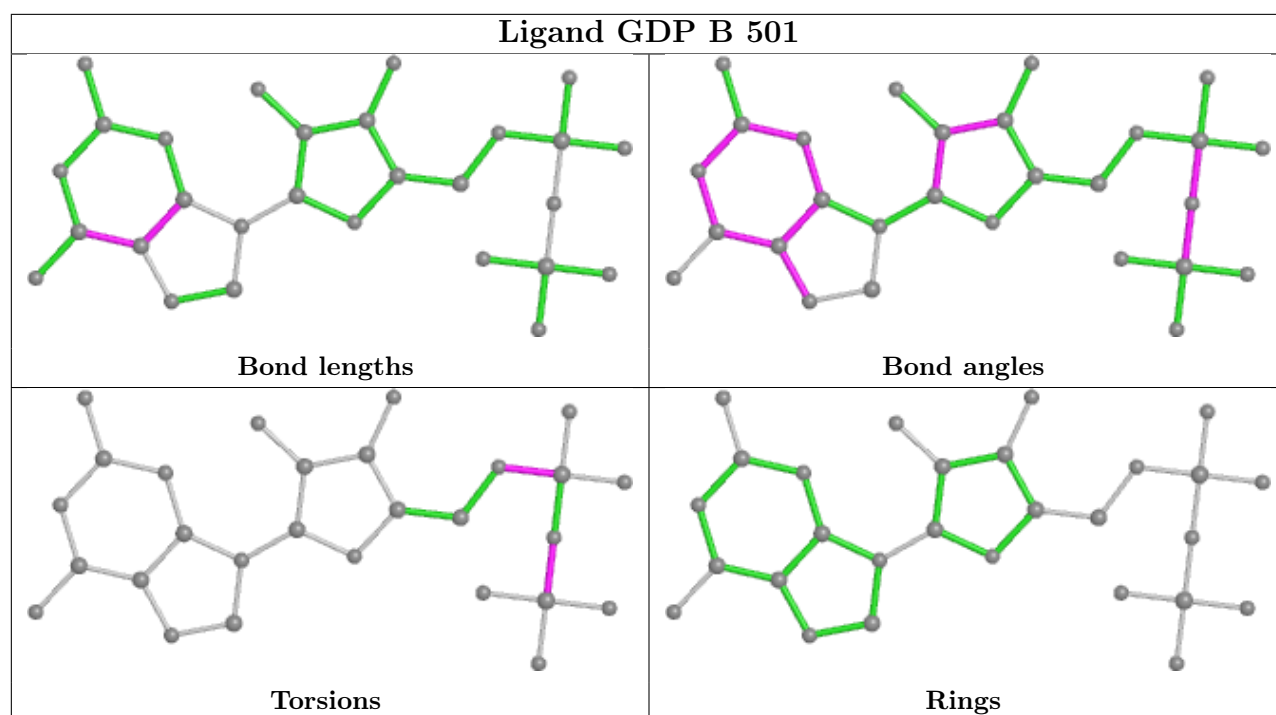


Ligand ACP F 401



Ligand WZ7 B 505





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.61	45 (10%) 6 3	81, 105, 151, 226	0
1	C	440/451 (97%)	0.43	25 (5%) 23 15	72, 91, 124, 170	0
2	B	425/445 (95%)	0.50	25 (5%) 22 14	74, 98, 154, 192	3 (0%)
2	D	431/445 (96%)	0.58	33 (7%) 13 7	91, 119, 160, 211	5 (1%)
3	E	123/143 (86%)	0.67	15 (12%) 4 2	95, 126, 172, 214	0
4	F	352/384 (91%)	0.44	23 (6%) 18 11	107, 147, 212, 257	0
All	All	2209/2319 (95%)	0.52	166 (7%) 14 8	72, 111, 175, 257	8 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	276	THR	8.7
3	E	6	MET	7.0
2	D	299	LYS	6.6
4	F	240	LEU	6.3
2	D	280	SER	6.2
3	E	26	PRO	6.1
3	E	27	PRO	5.5
2	D	277	SER	5.4
3	E	25	LYS	5.2
3	E	24	LEU	5.1
1	A	349	THR	4.9
2	D	217	LEU	4.8
2	D	275	LEU	4.7
1	A	86	LEU	4.6
1	A	342	GLN	4.4
1	C	368	LEU	4.4
1	A	348	PRO	4.3
1	A	312	TYR	4.3
2	B	332	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	4.1
2	D	278	ARG	4.0
2	D	218	LYS	4.0
1	A	344	VAL	3.9
2	D	281	GLN	3.9
4	F	243	HIS	3.8
2	B	337	ASN	3.8
4	F	314	LEU	3.8
1	A	351	PHE	3.6
1	A	317	LEU	3.6
1	C	230	LEU	3.5
2	D	248	LEU	3.5
2	B	336	GLN	3.5
4	F	234	GLN	3.4
4	F	169	LEU	3.4
1	A	340	SER	3.3
4	F	320	MET	3.2
1	A	316	CYS	3.2
2	B	333	LEU	3.2
1	C	4[A]	CYS	3.2
2	D	172	MET	3.2
1	C	179	THR	3.2
2	B	285	ALA	3.1
1	A	315	CYS	3.1
1	C	285	GLN	3.1
2	D	371	LEU	3.1
4	F	206	LEU	3.0
1	A	87	PHE	3.0
2	D	343	PHE	3.0
1	A	378	LEU	3.0
4	F	182	ILE	3.0
1	A	436	GLY	2.9
2	B	319	PHE	2.9
2	B	372	LYS	2.9
1	A	335	ILE	2.9
4	F	143	GLU	2.9
3	E	54	LEU	2.9
4	F	199	PHE	2.8
1	A	311	LYS	2.8
1	C	163	LYS	2.8
1	A	26	LEU	2.8
2	B	59	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	329	LEU	2.8
4	F	71	LEU	2.8
1	A	313	MET	2.8
1	A	382	THR	2.8
2	D	279	GLY	2.7
2	B	286	LEU	2.7
2	B	373	MET	2.7
1	C	276	ILE	2.7
1	A	270	ALA	2.7
4	F	338	CYS	2.7
1	C	296	PHE	2.7
2	D	272	PHE	2.7
1	A	296	PHE	2.7
1	A	339	ARG	2.6
1	C	87	PHE	2.6
3	E	115	HIS	2.6
1	C	275	VAL	2.6
1	C	339	ARG	2.6
3	E	28	SER	2.6
4	F	141	GLY	2.5
1	C	5	ILE	2.5
1	C	286	LEU	2.5
2	D	219	LEU	2.5
2	B	203	CYS	2.5
1	A	176	GLN	2.5
2	D	197	ASN	2.5
2	B	284	ARG	2.5
4	F	142	ARG	2.5
1	C	357	TYR	2.5
1	A	167	LEU	2.5
2	D	408	TYR	2.5
1	A	347	CYS	2.4
2	B	52	TYR	2.4
4	F	315	PHE	2.4
2	D	42	LEU	2.4
3	E	23	ILE	2.4
3	E	116	LEU	2.4
2	D	274	PRO	2.4
1	A	200	CYS	2.4
2	D	215	ARG	2.4
1	C	293	ASN	2.4
2	D	249	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	98	TYR	2.4
2	D	250	ALA	2.4
1	A	137	VAL	2.4
2	D	302	MET	2.4
1	A	269	LEU	2.4
2	D	195	VAL	2.3
1	A	202	PHE	2.3
3	E	22	VAL	2.3
1	A	357	TYR	2.3
1	A	141	PHE	2.3
4	F	186	LEU	2.3
1	A	337	THR	2.3
1	A	380	ASN	2.3
2	D	332	MET	2.3
2	B	318	ILE	2.3
4	F	39	LEU	2.3
1	A	88	HIS	2.3
1	A	438	ASP	2.3
2	B	325	MET	2.2
2	B	292	THR	2.2
1	A	314	ALA	2.2
1	C	302	MET	2.2
1	C	341	ILE	2.2
1	C	128	GLN	2.2
1	C	7	ILE	2.2
2	B	291	LEU	2.2
3	E	59	GLU	2.2
1	A	149	PHE	2.2
2	D	216	THR	2.2
1	A	377	MET	2.2
1	C	136	LEU	2.2
2	B	316	ALA	2.2
2	B	340	SER	2.2
2	B	66	ILE	2.1
1	A	112	LYS	2.1
1	A	332	ILE	2.1
1	C	281	ALA	2.1
1	C	279	GLU	2.1
1	A	68	VAL	2.1
1	C	135	PHE	2.1
4	F	20	LEU	2.1
2	B	384	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	308	ARG	2.1
3	E	8	VAL	2.1
1	A	169	PHE	2.1
2	B	313	LEU	2.1
2	B	432	TYR	2.1
3	E	76	ARG	2.1
2	B	276	THR	2.1
1	A	65	ALA	2.1
2	D	387	LEU	2.1
4	F	204	TRP	2.1
1	A	262	TYR	2.1
1	C	272	TYR	2.1
2	D	182	VAL	2.1
2	D	425	MET	2.1
2	D	204	ILE	2.0
3	E	50	ILE	2.0
4	F	302	ILE	2.0
2	B	281	GLN	2.0
4	F	339	ALA	2.0
2	D	432	TYR	2.0
1	C	370	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

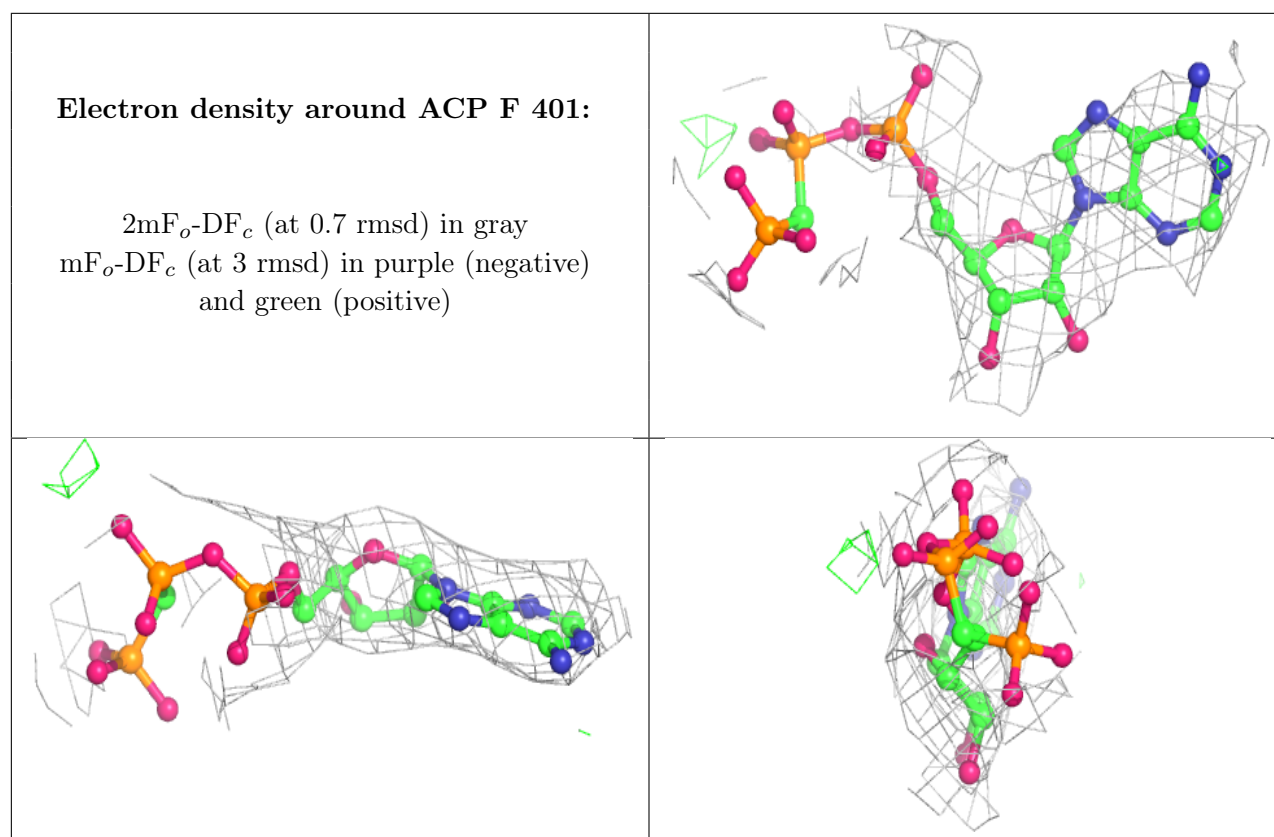
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	A	504	1/1	0.72	0.15	129,129,129,129	0
9	MES	B	504	12/12	0.78	0.27	118,124,139,148	0

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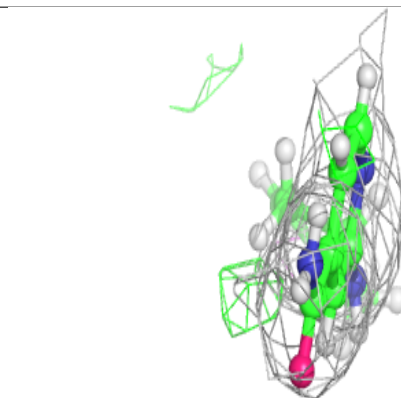
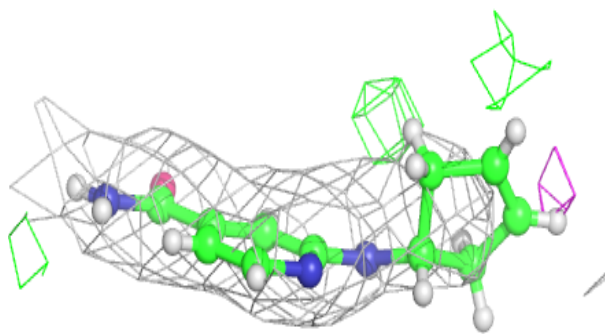
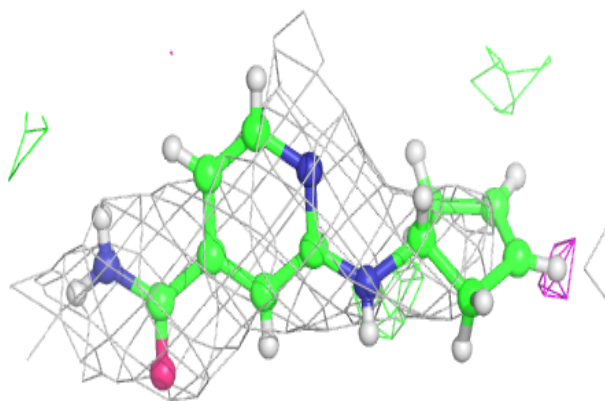
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	B	503	1/1	0.81	0.13	129,129,129,129	0
6	MG	D	502	1/1	0.87	0.10	114,114,114,114	0
11	ACP	F	401	31/31	0.87	0.15	145,158,167,178	0
10	WZ7	B	505	15/15	0.89	0.43	85,105,127,127	28
7	CA	A	503	1/1	0.92	0.15	134,134,134,134	0
6	MG	F	402	1/1	0.95	0.16	141,141,141,141	0
6	MG	B	502	1/1	0.95	0.19	96,96,96,96	0
8	GDP	D	501	28/28	0.95	0.20	104,112,118,124	0
5	GTP	A	501	32/32	0.97	0.18	75,82,90,95	0
5	GTP	C	501	32/32	0.97	0.21	74,80,90,92	0
7	CA	C	503	1/1	0.98	0.19	104,104,104,104	0
8	GDP	B	501	28/28	0.98	0.17	75,83,88,89	0
6	MG	C	502	1/1	0.98	0.19	87,87,87,87	0
6	MG	A	502	1/1	0.99	0.24	86,86,86,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

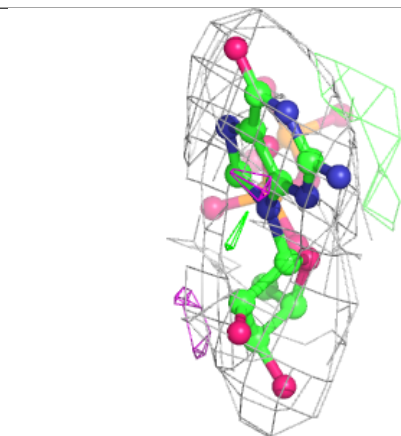
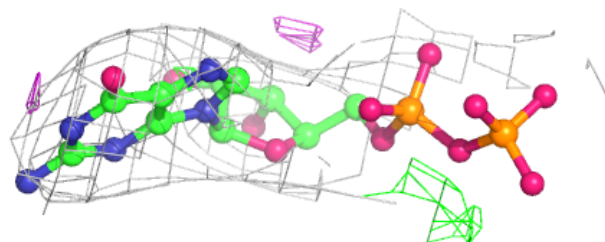
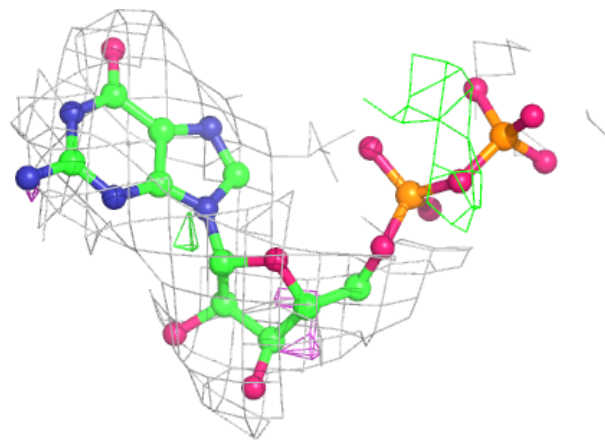


Electron density around WZ7 B 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

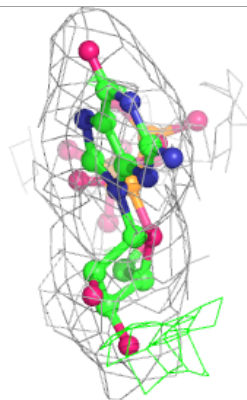
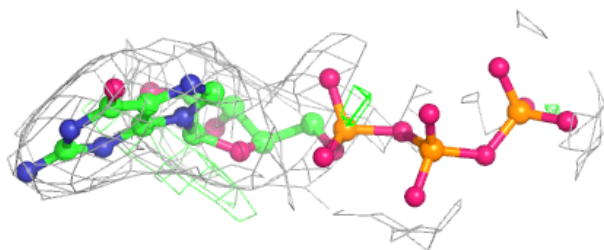
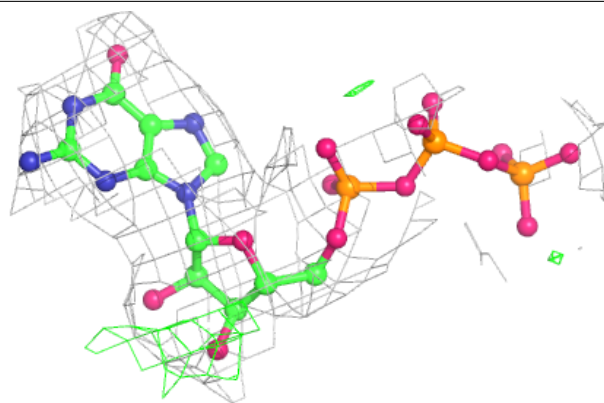
**Electron density around GDP D 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

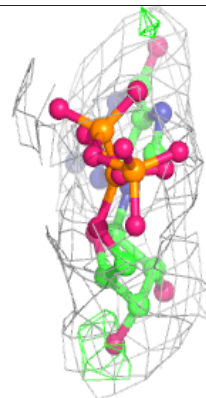
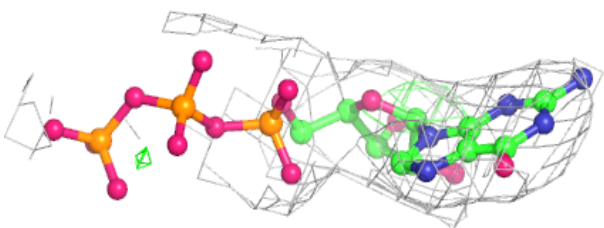
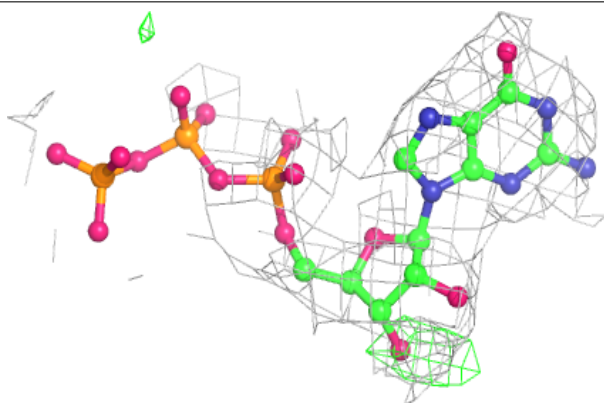


Electron density around GTP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

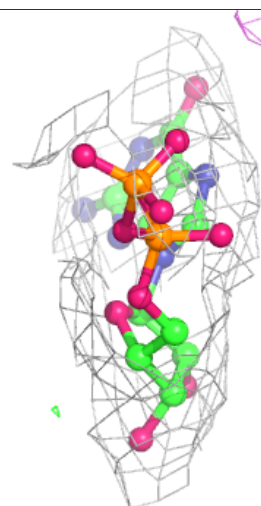
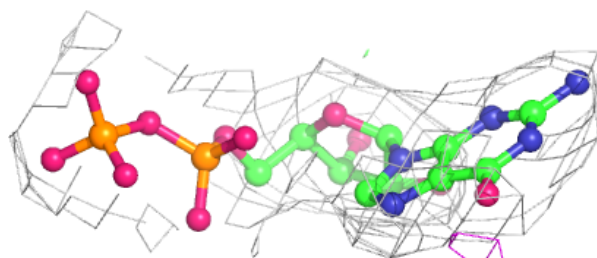
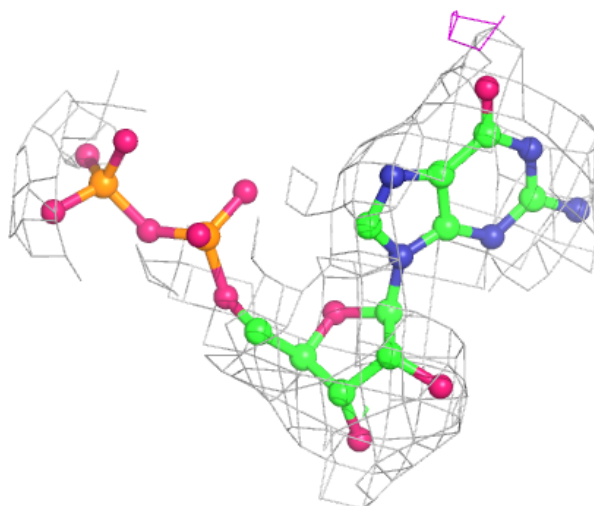
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.